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Wigner Representation of Quantum Operators and Its Applications to Electrons in a Magnetic Field

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The Wigner representation $F_s(p, q)$ of a quantum operator $F(\boldsymbol{p}, \boldsymbol{q})$ is defined by $F_s(p, q)=h\,\mathrm{Tr}\,F(\boldsymbol{p}, \boldsymbol{q})\Delta(p-\boldsymbol{p}, q-\boldsymbol{q})$ where Δ is a quantum analogue of a delta function in the phase space. This gives in particular the Wigner distribution function for a density operator. Basic theorems are summarized for the computation rules for quantummechanical operators in the Wigner representation. This is applied, in particular, to electrons in a magnetic field, for which a Wigner d. f. is introduced to describe the distribution of physical momenta $\vec{\pi}=m\vec{v}$, $\vec{v}$ being the velocity, and the position x. This description has the advantage to avoid the use of a vector potential and so to be gauge-independent. As examples of application, the diamagnetism and the Hall effect are briefly treated. Further applications of this treatment will be published later.

§ 1. Introduction

Many years ago, Wigner[1)] introduced into the quantum mechanics a phase-space distribution function which is an analogue to the distribution function of classical statistical mechanics and is called the Wigner distribution function (abbreviated in the following as Wigner d. f.). A Wigner d. f. has no definite sign unlike usual distribution functions, but nevertheless it provides a nice way of formulating quantum mechanics as a probabilistic theory. This point of view was extensively examined by Moyal[2)]. For a practical purpose of computation, Wigner distribution functions are particularly useful in order to obtain quantum corrections to classical formulae, because it gives a systematic method of expanding physical quantities in terms of $\hbar$, or the value of the non-commuting variables. Thus, Wigner d. f. has been extensively used in the theories of gaseous and liquid systems[3)]. Now, similar applications can be made for treating electrons in a magnetic field. If the magnetic field H lies in the z-direction and is uniform in space, the physical momenta,

$$\pi_x=mv_x, \quad \pi_y=mv_y$$

m being the mass and v_x and v_y, the velocity components, have the commutator

$$[\pi_x, \pi_y]=-\frac{\hbar eH}{ci}\equiv-\frac{\hbar'}{i}, \quad \hbar'\equiv\frac{\hbar eH}{c}.$$

If it is desired to obtain an expansion in terms of H or $\hbar'$, then the Wigner d. f. will be found to be a very useful tool. The purpose of the present paper is to show a few examples of such application of Wigner d. f.[4)] However, considering the fact that only few literatures are available for the reference of basic theorems concerning the Wigner d. f., Part I of this paper is devoted to a brief summary of such theorems, some of which are presented there in somewhat new forms although most of them have been already known.

Part I. Wigner Representation

§ 2. Symmetrized Operators

For simplicity's sake, most of the following formulae are written for a system with only one degree of freedom, the cannonical variables of which will be denoted by p and q, but they apply to many degrees of freedom with obvious modifications. Gothic letters, as $\boldsymbol{p}$ or $\boldsymbol{q}$, mean quantum-mechanical operators and corresponding classical variables are denoted by p or q.

A function of $\boldsymbol{p}$ and $\boldsymbol{q}$, $A_s(\boldsymbol{p}, \boldsymbol{q})$, is said to be a symmetrized operator if it has the form

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$$A_s(\boldsymbol{p},\boldsymbol{q})=\iint_{-\infty}^{\infty} d\xi d\eta G_A(\xi,\eta)\exp i(\xi\boldsymbol{p}+\eta\boldsymbol{q}) \quad (2.1)$$

because, as evident from the definition of the exponential function, any product of $\boldsymbol{p}$ and $\boldsymbol{q}$ in this function is totally symmetrized with respect to their order of multiplication. Generally speaking, a quantum mechanical operator is not necessarity symmetrized, but it can be expressed in terms of symmetrized operators. For instance in

$$\boldsymbol{pq}=\frac{1}{2}(\boldsymbol{pq}+\boldsymbol{qp})+\frac{\hbar}{2i}\equiv\{\boldsymbol{pq}\}_s+\frac{\hbar}{2i},$$

the left hand side is not symmetrized, whereas the right hand side is so. A prescription how to rewrite an operator function, $F(\boldsymbol{p},\boldsymbol{q})$ into a symmetrized form $F_s(\boldsymbol{p},\boldsymbol{q})$ is given by the following theorem. Other equivalent methods will be given later.

Theorem 1. For a given operator function, $F(\boldsymbol{p},\boldsymbol{q})$, define $G(\xi,\eta)$ by

$$G(\xi,\eta)=\mathrm{Tr}\,F(\boldsymbol{p},\boldsymbol{q})\exp\{-i(\xi\boldsymbol{p}+\eta\boldsymbol{q})\}, \quad (2.2)$$

$$\equiv\int_{-\infty}^{\infty}\langle q'-\hbar\xi|F|q'\rangle dq'\exp\left\{-i\eta\left(q'-\frac{\hbar\xi}{2}\right)\right\}, \quad (2.3)$$

where (2.3) is an explicit form of (2.2) in the q-representation. Then the operator $F(\boldsymbol{p},\boldsymbol{q})$ can be expressed by

$$F(\boldsymbol{p},\boldsymbol{q})=F_s(\boldsymbol{p},\boldsymbol{q})$$
$$=\frac{\hbar}{2\pi}\iint_{-\infty}^{\infty}G(\xi,\eta)d\xi d\eta\exp i(\xi\boldsymbol{p}+\eta\boldsymbol{q}), \quad (2.4)$$

which gives its symmetrized form.

This theorem may be stated in an alternative form:

Theorem 2. For a given operator function, $F(\boldsymbol{p},\boldsymbol{q})$, define

$$F_s(p,q)=h\,\mathrm{Tr}\,F(\boldsymbol{p},\boldsymbol{q})\Delta(p-\boldsymbol{p},q-\boldsymbol{q}) \quad (2.5)$$

$$=\int\left\langle q-\frac{\hbar\xi}{2}|F|q+\frac{\hbar\xi}{2}\right\rangle e^{i\xi p}\hbar d\xi. \quad (2.6)$$

Then we have

$$F(\boldsymbol{p},\boldsymbol{q})=F_s(\boldsymbol{p},\boldsymbol{q})$$
$$=\iint dp dq F_s(p,q)\Delta(p-\boldsymbol{p},q-\boldsymbol{q}), \quad (2.7)$$

where

$$\Delta(p-\boldsymbol{p},q-\boldsymbol{q})$$
$$=\frac{1}{(2\pi)^2}\iint_{-\infty}^{\infty}\exp i(\xi(p-\boldsymbol{p})+\eta(q-\boldsymbol{q})). \quad (2.8)$$

is a quantum-analogue of a delta function in the phase space.

For the proof of the theorems, we refer to a lemma which is due to Moyal:

Lemma

$$\exp i(\xi\boldsymbol{p}+\eta\boldsymbol{q})=e^{i\xi p}e^{i\eta q}e^{-i\hbar\xi\eta/2}=e^{i\eta q}e^{i\xi p}e^{i\hbar\xi\eta/2}$$
$$=e^{i\xi p/2}e^{i\eta q}e^{i\xi p/2}=e^{i\eta q/2}e^{i\xi p}e^{i\eta q/2}, \quad (2.9)$$

or in the q-representation,

$$\langle q'|\exp i(\xi\boldsymbol{p}+\eta\boldsymbol{q})|q''\rangle$$
$$=\exp i\eta\left(q'+\frac{1}{2}\hbar\xi\right)\delta(q'+\hbar\xi-q''). \quad (2.10)$$

These are easily obtained from the commutation rule of $\boldsymbol{p}$ and $\boldsymbol{q}$.

By Eq. (2.10), (2.2) gives (2.3), which is inserted into (2.4) to give

$$\langle q'|F_s(\boldsymbol{p},\boldsymbol{q})|q''\rangle$$
$$=\frac{\hbar}{2\pi}\iint_{-\infty}^{\infty}\exp\left\{i\eta\left(q'+\frac{\hbar}{2}\xi\right)\right\}\delta(q'+\hbar\xi-q'')d\xi d\eta$$
$$\times\langle q'''-\hbar\xi|F|q'''\rangle dq'''\exp\left\{-i\eta\left(q'''-\frac{\hbar}{2}\xi\right)\right\}$$
$$=\langle q'|F|q''\rangle.$$

This establishes the equality of $F(\boldsymbol{p},\boldsymbol{q})$ and $F_s(\boldsymbol{p},\boldsymbol{q})$, the latter being symmetrized by its definition (2.4).

By Eqs. (2.2) and (2.8), $F_s(p,q)$ is in fact equal to

$$F_s(q,q)=\frac{\hbar}{2\pi}\iint_{-\infty}^{\infty}G(\xi,\eta)d\xi d\eta\, e^{i(\xi p+\eta p)}. \quad (2.11)$$

Thus Eq. (2.7) is equivalent to Eq. (2.4). Equation (2.6) follows from (2.3) and (2.11).

Now, let ρ be a density operator to describe a statistical property of a quantum system which may be in a pure or mixed state. Then we have:

Theorem 3. The Wigner d. f. for the density operator ρ is defined by

$$f(p,q)=h\langle\Delta(p-\boldsymbol{p},q-\boldsymbol{q})\rangle$$
$$\equiv h\,\mathrm{Tr}\,\rho\Delta(p-\boldsymbol{p},q-\boldsymbol{q}). \quad (2.12)$$

Then ρ is represented by

$$\rho(\boldsymbol{p},\boldsymbol{q})=\iint dp dq f(p,q)\Delta(p-\boldsymbol{p},q-\boldsymbol{q}). \quad (2.13)$$

This is a direct consequence of the preceding theorems. Equation (2.12) is equivalent to the more familar definition of Wigner d. f.,

$$f(p,\ q)=\int\left\langle q-\frac{r}{2}|\rho|q+\frac{r}{2}\right\rangle e^{irp/\hbar}dr\ , \quad (2.14)$$

as is seen at once from Eq. (2.6). This can be obtained by the matrix representation of Δ,

$$\langle q'|\Delta(p-\boldsymbol{p},\ q-\boldsymbol{q})|q''\rangle$$
$$=\frac{1}{2\pi}\int d\xi\delta\left(q'-q+\frac{\hbar\xi}{2}\right)\delta(q'-q''-\hbar\xi)e^{-i\xi p}, \quad (2.15)$$

which follows from the lemma (2.10). Equation (2.15) also gives

$$\mathrm{Tr}\ \Delta(p-\boldsymbol{p},\ q-\boldsymbol{q})=\frac{1}{h}\ , \quad (2.16)$$

and

$$\iint dpdq\Delta(p-\boldsymbol{p},\ q-\boldsymbol{q})=\boldsymbol{1}\ . \quad (2.17)$$

Accordingly the normalization

$$\mathrm{Tr}\ \rho(\boldsymbol{p},\ \boldsymbol{q})=\frac{1}{h}\iint dpdqf(p,\ q)\ , \quad (2.18)$$

is proved.

It should be remembered that a density operator $\rho(\boldsymbol{p},\ \boldsymbol{q})$, for example,

$$\rho(\boldsymbol{p},\ \boldsymbol{q})=e^{-\beta\mathscr{H}(\boldsymbol{p},\ \boldsymbol{q})},$$

is not symmetrized. Therefore the calculation of the corresponding Wigner d. f. is equivalent to rewriting it into a *symmetrized form*.

§ 3. Wigner Operators

We have seen that a phase function, $F_s(p,\ q)$, is found for a given operator $F(\boldsymbol{p},\ \boldsymbol{q})$ by Eq. (2.5). This is generally a one-to-one correspondence, so that $F_s(p,\ q)$ may be regarded as a representation of the operator $F(\boldsymbol{p},\ \boldsymbol{q})$, which will be called the *Wigner representation* of F. The functional form of $F_s(p,\ q)$ is identical with that of $F(\boldsymbol{p},\ \boldsymbol{q})$ if and only if the latter is already symmetrized. Generally, a product of two operators, $\boldsymbol{A}$ and $\boldsymbol{B}$, is not symmetrized even when they are symmetrized. Thus, we have to find the rule to construct the Wigner representation of such a product from the known Wigner representations of $\boldsymbol{A}$ and $\boldsymbol{B}$. For this purpose, we introduce differential operators, which will be called *Wigner operators*, by the following definitions:

$$A_w\equiv A_s\left(p+\frac{\hbar}{2i}\frac{\partial}{\partial q},\quad q-\frac{\hbar}{2i}\frac{\partial}{\partial p}\right)$$
$$=\frac{\hbar}{2\pi}\iint_{-\infty}^{\infty}d\xi d\eta G_A(\xi,\ \eta)$$
$$\times\exp i\left\{\xi\left(p+\frac{\hbar}{2i}\frac{\partial}{\partial q}\right)+\eta\left(q-\frac{\hbar}{2i}\frac{\partial}{\partial p}\right)\right\} \quad (3.1)$$

$$\bar{A}_w\equiv A_s\left(p-\frac{\hbar}{2i}\frac{\partial}{\partial q},\quad q+\frac{\hbar}{2i}\frac{\partial}{\partial p}\right)$$
$$=\frac{\hbar}{2\pi}\iint_{-\infty}^{\infty}d\xi d\eta G_A(\xi,\ \eta)$$
$$\times\exp i\left\{\xi\left(p-\frac{\hbar}{2i}\frac{\partial}{\partial q}\right)+\eta\left(q+\frac{\hbar}{2i}\frac{\partial}{\partial p}\right)\right\}, \quad (3.2)$$

where

$$G_A(\xi,\ \eta)=\frac{1}{h}\iint_{-\infty}^{\infty}A_s(p,\ q)e^{-i(\xi p+\eta q)}dpdq$$
$$=\mathrm{Tr}\ A(\boldsymbol{p},\ \boldsymbol{q})\exp\{-i(\xi\boldsymbol{q}+\eta\boldsymbol{q})\}\ . \quad (3.3)$$

By Eq. (2.11), $A_s(p,\ q)$ is the Wigner representation of the operator, $\boldsymbol{A}=A(\boldsymbol{p},\ \boldsymbol{q})$. We then have:

Theorem 4. Let $A_s(p,\ q)$ and $B_s(p,\ q)$ be the Wigner representations of the operators $\boldsymbol{A}$ and $\boldsymbol{B}$. Then

$$A_w\cdot 1=\bar{A}_w\cdot 1=A_s(p,\ q)\ , \quad (3.4)$$

and

Wigner representation of $\boldsymbol{AB}$

$$=A_wB_w\cdot 1=\bar{B}_wA_w\cdot 1\ . \quad (3.5)$$

For the proof, we note the identities

$$\exp i(\xi_1\boldsymbol{p}+\eta_1\boldsymbol{q})\exp i(\xi_2\boldsymbol{p}+\eta_2\boldsymbol{q})$$
$$=\exp\left[i\{(\xi_1+\xi_2)\boldsymbol{p}+(\eta_1+\eta_2)\boldsymbol{q}\}+\frac{i\hbar}{2}(\xi_1\eta_2-\eta_1\xi_2)\right], \quad (3.6)$$

$$\exp i\left\{\xi\left(p+\frac{\hbar}{2i}\frac{\partial}{\partial q}\right)+\eta\left(q-\frac{\hbar}{2i}\frac{\partial}{\partial q}\right)\right\},$$
$$=\exp i(\xi p+\eta q)\exp\frac{\hbar}{2}\left(\xi\frac{\partial}{\partial q}-\eta\frac{\partial}{\partial p}\right), \quad (3.7a)$$
$$=\exp\frac{\hbar}{2}\left(\xi\frac{\partial}{\partial q}-\eta\frac{\partial}{\partial p}\right)\exp i(\xi p+\eta q)\ , \quad (3.7b)$$

and

$$\exp i\left\{\xi_1\left(p+\frac{\hbar}{2i}\frac{\partial}{\partial q}\right)+\eta_1\left(q-\frac{\hbar}{2i}\frac{\partial}{\partial p}\right)\right\}$$
$$\times\exp i\left\{\xi_2\left(p+\frac{\hbar}{2i}\frac{\partial}{\partial q}\right)+\eta_2\left(q-\frac{\hbar}{2i}\frac{\partial}{\partial p}\right)\right\}$$
$$=\exp i\left\{(\xi_1+\xi_2)\left(p+\frac{\hbar}{2i}\frac{\partial}{\partial q}\right)\right.$$
$$\left.+(\eta_1+\eta_2)\left(q-\frac{\hbar}{2i}\frac{\partial}{\partial p}\right)\right\}\exp\frac{i\hbar}{2}(\xi_1\eta_2-\eta_1\xi_2)\ , \quad (3.8)$$

Equation (3.6) follows from the lemma (2.9), whereas (3.7) and (3.8) follow from a similar identity,

$$\exp\left(ax+b\frac{\partial}{\partial x}\right)=e^{ax}e^{b(\partial/\partial x)}e^{ab/2}$$
$$=e^{b(\partial/\partial x)}e^{ax}e^{-ab/2}\,. \qquad (3.9)$$

Equation (3.4) is easily seen from the definitions of A_w and $\bar{A}_w$, (3.1) and (3.2), by using Eq. (3.7a); namely,

$$A_w\cdot 1=\frac{\hbar}{2\pi}\iint_{-\infty}^{\infty}d\xi d\eta G_A(\xi,\eta)\exp i(\xi p+\eta q)$$
$$\times\exp\frac{\hbar}{2}\left(\xi\frac{\partial}{\partial q}-\eta\frac{\partial}{\partial p}\right)\cdot 1$$
$$=\frac{\hbar}{2\pi}\iint_{-\infty}^{\infty}d\xi d\eta G_A(\xi,\eta)$$
$$\times\exp i(\xi p+\eta q)=A_s(p,q)\,,$$

and similarly for $\bar{A}_w\cdot 1$. In order to show (3.5), we observe first that Eqs. (2.4) and (3.6) give

$$\boldsymbol{AB}=\left(\frac{\hbar}{2\pi}\right)^2\iiiint_{-\infty}^{\infty}G_A(\xi_1,\eta_1)G_B(\xi_2,\eta_2)d\xi_1d\eta_1d\xi_2d\eta_2$$
$$\times\exp\left[\{i(\xi_1+\xi_2)\boldsymbol{p}+(\eta_1+\eta_2)\boldsymbol{q}\}+\frac{i\hbar}{2}(\xi_1\eta_2-\eta_1\xi_2)\right], \qquad (3.10)$$

which shows that

Wigner representation of $\boldsymbol{AB}$

$$=\left(\frac{\hbar}{2\pi}\right)^2\iiiint_{-\infty}^{\infty}G_A(\xi_1,\eta_1)G_B(\xi_2,\eta_2)d\xi_1d\eta_1d\xi_2d\eta_2$$
$$\times\exp\left[i(\xi_1+\xi_2)p+(\eta_1+\eta_2)q\}+\frac{i\hbar}{2}(\xi_1\eta_2-\eta_1\xi_2)\right]. \qquad (3.11)$$

Now, use Eq. (3.1) for explicit expressions of A_w and B_w, Eq. (3.8) for the product of exponential operators and Eq. (3.7a) for operating the differential operator on 1; then one easily sees that $A_wB_w\cdot 1$ is in fact equal to (3.11). By a similar calculation the second equality in (3.5) can be established. This last point can, however, be stated by a more general theorem; i. e.,

Theorem 5. For Wigner operators defined by (3.1) and (3.2), we have the identity,

$$A_w\bar{B}_w=\bar{B}_wA_w\,,\quad\text{or } [A_w,\bar{B}_w]=0\,. \qquad (3.12)$$

This follows from the identity,

$$\left[\exp i\left\{\xi_1\left(p+\frac{\hbar}{2i}\frac{\partial}{\partial q}\right)+\eta_1\left(q-\frac{\hbar}{2i}\frac{\partial}{\partial q}\right)\right\},\right.$$
$$\left.\exp i\left\{\xi_2\left(p-\frac{\hbar}{2i}\frac{\partial}{\partial p}\right)+\eta_2\left(q+\frac{\hbar}{2i}\frac{\partial}{\partial p}\right)\right\}\right]=0. \qquad (3.13)$$

This is proved by repeated use of the relations (3.7a, b) and (3.9). Therefore, Eq. (3.5) is obtained as

$$A_wB_w\cdot 1=A^H\bar{B}_w\cdot 1=\bar{B}_wA_w\cdot 1\,. \qquad (3.14)$$

This means that the product of two operators, $\boldsymbol{AB}$, can be interpreted into the Wigner representation in two ways (which are of course equivalent to one another); namely, if $\boldsymbol{A}$ multiplies $\boldsymbol{B}$ from the left, A_w operates on B_w; if $\boldsymbol{B}$ multiplies $\boldsymbol{A}$ from the right, $\bar{B}_w$ operates on A_w. Therefore, we may call A_w, defined by (3.1), a *left Wigner operator*, and $\bar{A}_w$, defined by (3.2) a *right Wigner operator*. For example,

$$A_wB_wC_wD_w\cdot 1=A_wB_w\bar{D}_wC_w\cdot 1=\cdots$$
$$=\bar{D}_wA_wB_wC_w\cdot 1=\bar{D}_wA_wC_w\bar{B}_w\cdot 1=\cdots$$
$$=\bar{D}_wC_w\bar{B}_w\bar{A}_w\cdot 1\,, \qquad (3.15)$$

is the Wigner representation of the operator product, $\boldsymbol{ABCD}$; all of the expressions in Eq. (3.15) give the same result, because they merely correspond to different interpretation of multiplication from the left or from the right.

If an operator $F(\boldsymbol{p},\boldsymbol{q})$ is given in the form (2.7), its trace is obtained by

$$\mathrm{Tr}\,F(\boldsymbol{p},\boldsymbol{q})=\frac{1}{h}\iint dpdqF_s(p,q)\,, \qquad (3.16)$$

because of Eq. (2.16). Thus, taking the trace of a quantum operator is the phase-space integration of its Wigner representation. For this we have the basic theorem:

Theorem 6. The trace of $\boldsymbol{AB}$, if it exists, is given by

$$\mathrm{Tr}\,\boldsymbol{AB}=\frac{1}{h}\iint dpdqA_s(p,q)B_s(p,q)\,, \qquad (3.17)$$

in the Wigner representation. This is proved as follows;

$$\mathrm{Tr}\,\boldsymbol{AB}=\frac{1}{h}\iint dpdqA_wB_w\cdot 1$$
$$=\frac{1}{h}\iint dp\,dq\frac{\hbar}{2\pi}\iint d\xi d\eta$$
$$\times\exp\frac{\hbar}{2}\left(\xi\frac{\partial}{\partial q}-\eta\frac{\partial}{\partial p}\right)\exp i(\xi p+\eta q)$$
$$\times G_A(\xi,\eta)B_s(p,q)\,,$$

$$=\frac{1}{h}\iint dp\,dq\frac{\hbar}{2\pi}\iint d\xi d\eta e^{i(\xi p+\eta q)}G_A(\xi,\eta)B_s(p,q)\,,$$
$$=\frac{1}{h}\iint dp dq A_s(p,q)B_s(p,q)\,.$$

The second line is obtained from the first line, which follows from (3.16) and (3.5), by writing A_w in the form (3.2) with the transformation (3.7b) and by using the relation (3.4) for $B_w\cdot 1$. The third line is the result of partial integration, the boundary values being assumed to vanish.

By the theorems 4, 5, 6, Eq. (3.15) and by the cyclic property of trace, the trace of a product, $\boldsymbol{ABCD}$, for example, can be expressed in various forms, all of which give of course the identical value provided that the trace does converge. Thus, for example, we may write

$$\begin{aligned}\mathrm{Tr}\,\boldsymbol{ABCD}&=\frac{1}{h}\iint dp dq A_w B_w C_w D_s(p,q)\\&=\frac{1}{h}\iint dp dq A_s(p,q)B_w C_w D_s(p,q)\\&=\frac{1}{h}\iint dp dq(\bar{B}_w A_s(p,q))(C_w D_s(p,q))\\&=\frac{1}{h}\iint dp dq(A_w B_s(p,q))(C_w D_s(p,q))\\&=\frac{1}{h}\iint dp dq(D_w A_s(p,q))(B_w C_s(p,q))\,,\ \text{etc.}\end{aligned}\tag{3.18}$$

There exists another transformation which gives different appearance of the expression keeping, however, the value of the trace invariant. This is shown by

$$\begin{aligned}\mathrm{Tr}\,\boldsymbol{AB}\cdots\boldsymbol{D}&=\frac{1}{h}\iint A_w B_w\cdots D_w\cdot 1\\&=\frac{1}{h}\iint dp dq\exp\left(-\frac{\varepsilon\hbar}{2i}\frac{\partial^2}{\partial p\,\partial q}\right)\\&\quad\times\exp\left(\frac{\varepsilon\hbar}{2i}\frac{\partial^2}{\partial p\,\partial q}\right)A_w\cdots D_w\exp\left(-\frac{\varepsilon\hbar}{2i}\frac{\partial^2}{\partial p\,\partial q}\right)\cdot 1\\&=\frac{1}{h}\iint dp dq A_w^{\varepsilon}\cdots D_w^{\varepsilon}1\end{aligned}\tag{3.19}$$

where

$$\begin{aligned}A_w^{\varepsilon}&=\exp\left(\frac{\varepsilon\hbar}{2i}\frac{\partial^2}{\partial p\,\partial q}\right)A_s\left(p+\frac{\hbar}{2i}\frac{\partial}{\partial q},\ q-\frac{\hbar}{2i}\frac{\partial}{\partial p}\right)\\&\quad\times\exp\left(-\frac{\varepsilon\hbar}{2i}\frac{\partial^2}{\partial p\,\partial q}\right)\\&=A_s\left(p+\frac{\hbar(1+\varepsilon)}{2i}\frac{\partial}{\partial q},\ q-\frac{\hbar(1-\varepsilon)}{2i}\frac{\partial}{\partial p}\right).\end{aligned}\tag{3.20}$$

The theorems and remarks mentioned above can be applied for calculations of statistical averages defined by a given density operator $\boldsymbol{\rho}$. Thus we can write

$$\langle\boldsymbol{A}\rangle=\mathrm{Tr}\,\boldsymbol{A\rho}=\frac{1}{h}\iint dp dq A_s(p,q)f(p,q)\,,\tag{3.21}$$

or more generally

$$\langle\boldsymbol{AB}\cdots\boldsymbol{D}\rangle\equiv\mathrm{Tr}\,\boldsymbol{AB}\cdots\boldsymbol{D\rho}=\frac{1}{h}\iint dp dq A_w B_w\cdots D_w f(p,q)\,,\tag{3.22}$$

where A_w, etc. are Wigner operators operating on the Wigner d. f.. By such relations as (3.18) and (3.19), the expression (3.22) may also be written in a number of different ways.

Finally, we remark

Theorem 7. The Wigner operator A_w defined by (3.1) may be written as

$$A_w=\exp\left\{\frac{\hbar}{2i}\left(\frac{\partial}{\partial p_A}\frac{\partial}{\partial q}-\frac{\partial}{\partial q_A}\frac{\partial}{\partial p}\right)\right\}A_s(p,q)\,,\tag{3.23}$$

where $\partial/\partial p_A$ or $\partial/\partial q_A$ means the differentiation of the function $A_s(p,q)$ while $\partial/\partial p$ or $\partial/\partial q$ operates on a function which follows after A_w; namely

$$A_w f(p,q)=\sum_{m,n}\frac{(-)^n\hbar^{n+m}}{m!n!(2i)^{n+m}}\frac{\partial^{n+m}A_s(p,q)}{\partial p^n\partial q^m}\frac{\partial^{n+m}f(p,q)}{\partial q^n\partial p^m}\,.\tag{3.24}$$

The differentiations of A_s and f can be separated in this way by virtue of the identity (3.7a).

§ 4. Equation of Motion and Bloch Equation

By the basic theorems given in the preceding sections, it is easy to interpret quantum-mechanical expressions for operators into the Wigner representation or to interpret expressions in the Wigner represetation back into more familiar quantum-operator expressions. In this way, one can choose either representation convenient of the purpose of calculation.

The equation of motion of the density matrix $\boldsymbol{\rho}$,

$$\frac{\partial\boldsymbol{\rho}}{\partial t}=\frac{1}{it}[\mathscr{H}(\boldsymbol{p},\boldsymbol{q},t),\boldsymbol{\rho}]\,,\tag{4.1}$$

is now read, in the Wigner representation, as

$$\frac{\partial f}{\partial t}=\frac{1}{i\hbar}(\mathscr{H}_w-\bar{\mathscr{H}}_w)f\equiv i\mathscr{L}f\ , \tag{4.2}$$

where $\mathscr{H}(\boldsymbol{p}, \boldsymbol{q}, t)$ is the Hamiltonian, which may explicitly depend on the time t, and $\mathscr{H}_w$ and $\bar{\mathscr{H}}_w$ are the corresponding Wigner operators. If $\mathscr{H}(\boldsymbol{p}, \boldsymbol{q}, t)$ is already a symmetrized operator, as it usually is, then the "Liouville operator" for the Wigner d. f. is given by

$$\begin{aligned} i\mathscr{L}&\equiv\frac{1}{i\hbar}\left\{\mathscr{H}\left(p+\frac{\hbar}{2i}\frac{\partial}{\partial q},\ q-\frac{\hbar}{2i}\frac{\partial}{\partial p},\ t\right)\right.\\ &\qquad\left.-\mathscr{H}\left(p-\frac{\hbar}{2i}\frac{\partial}{\partial q},\ q+\frac{\hbar}{2i}\frac{\partial}{\partial p},\ t\right)\right\}\\ &=\frac{1}{i\hbar}\{\mathscr{H}(p_w, q_w, t)-\mathscr{H}(\bar{p}_w, \bar{q}_w, t)\}\ . \end{aligned} \tag{4.3}$$

If this is expanded in a power series of $\hbar$ by the formula (3.24), the first term in $0(\hbar^0)$ is of course the classical Liouville operator, and the following terms appearing only in even powers of $\hbar$ give its quantum corrections.

Correspondingly, the Heisenberg equation of motion of a dynamical variable $\boldsymbol{A}=A(\boldsymbol{p}_t, \boldsymbol{q}_t)$,

$$\frac{d}{dt}A(\boldsymbol{p}_t, \boldsymbol{q}_t)=\frac{1}{i\hbar}[A(\boldsymbol{p}_t, \boldsymbol{q}_t),\ \mathscr{H}(\boldsymbol{p}_t, \boldsymbol{q}_t, t)] \tag{4.4}$$

is read as

$$\frac{d}{dt}A_s(p_t, q_t)=-i\mathscr{L}(p_t, q_t, t)A_s(p_t, q_t)\ , \tag{4.5}$$

where $\mathscr{L}(p_t, q_t, t)$ has the same functional form as (4.3). Obviously, in the classical limit of $\hbar\to 0$, Eq. (4.5) is identical with the classical equation of motion

$$\begin{aligned} \frac{d}{dt}A(p_t, q_t)&=-i\mathscr{L}_{\mathrm{cl}}(p_t, q_t, t)A(p_t, q_t)\\ &=\frac{\partial A}{\partial q_t}\frac{\partial\mathscr{H}}{\partial p_t}-\frac{\partial A}{\partial q_t}\frac{\partial\mathscr{H}}{\partial q_t}\ , \end{aligned} \tag{4.6}$$

which is equivalent to the Hamilton equation,

$$\dot{p}_t=-\frac{\partial}{\partial q_t}\mathscr{H}(p_t, q_t, t),\ \dot{q}=\frac{\partial}{\partial p_t}\mathscr{H}(p_t, q_t, t)\ , \tag{4.7}$$

because the phase function $A(p_t, q_t)$ depends on t through the temporal change of p_t and q_t, which is determined by (4.7) for a given initial condition, e. g. $p_0=p$, $q_0=q$. In the same way, Eq. (4.5) determines the temporal change of the Wigner representation of a quantum operator $A(\boldsymbol{p}_t, \boldsymbol{q}_t)$ which obeys Eq. (4.4) with the corresponding initial condition

$$A(\boldsymbol{p}_0, \boldsymbol{q}_0)=A(\boldsymbol{p}, \boldsymbol{q})\ .$$

The explicit time dependence of the Wigner representation,

$$A_s(p_t, q_t)=A(t;\ p, q)\ , \tag{4.8}$$

with the initial condition

$$A_s(0;\ p, q)=A_s(p, q)\ , \tag{4.9}$$

may be defined by

$$A_s(t;\ p, q)=h\operatorname{Tr}A(\boldsymbol{p}_t, \boldsymbol{q}_t)\Delta(p-\boldsymbol{p}, q-\boldsymbol{q})\ . \tag{4.10}$$

In particular,

$$\begin{aligned} p_t&=h\operatorname{Tr}\boldsymbol{p}_t\Delta(p-\boldsymbol{p},\ q-\boldsymbol{q})\ ,\\ q_t&=h\operatorname{Tr}\boldsymbol{q}_t\Delta(p-\boldsymbol{p},\ q-\boldsymbol{q})\ , \end{aligned} \tag{4.11}$$

give the Wigner representations of canonical variables with the initial condition, $p_0=p$, $q_0=q$. By differentiating Eq. (4.10) with respect to t and by using Eq. (4.4), (4.11) and the theorems 3 and 4, we derive

$$\frac{d}{dt}A_s(t;\ p, q)=-i\mathscr{L}(p_t, q_t, t)A_s(t;\ p, q)\ . \tag{4.12}$$

In particular, p_t and q_t defined by (4.11) satisfy

$$\frac{dp_t}{dt}=-i\mathscr{L}p_t\ ,\quad \frac{dq_t}{dt}=-i\mathscr{L}q_t\ . \tag{4.13}$$

This shows that the solution of (4.12) is given by (4.8). This can be directly seen by noticing that the formal solution of Eq. (4.12) can be written as

$$\begin{aligned} A_s(t;\ p, q)&=S(t)A_s(p, q)\\ &\equiv S(t)A_s(p, q)S(t)^{-1}\ , \end{aligned} \tag{4.14}$$

where

$$\begin{aligned} S(t)&=\exp_{\rightarrow}\left(-i\int_0^t\mathscr{L}(p, q, t')dt'\right)\\ \mathrm{S}(t)^{-1}&=\exp_{\leftarrow}\left(i\int_0^t\mathscr{L}(p, q, t')dt'\right)\ , \end{aligned} \tag{4.15}$$

are ordered exponential operators ordered chronologically as indicated by arrows. Since $\mathscr{L}$ is a differential operator, the last factor $\mathrm{S}^{-1}(t)$ of (4.4) results in 1. In the same way we have

$$\begin{aligned} p_t&=\mathrm{S}(t)p\equiv\mathrm{S}(t)p\mathrm{S}^{-1}(t)\\ q_t&=\mathrm{S}(t)q\equiv\mathrm{S}(t)q\mathrm{S}^{-1}(t)\\ \frac{\partial}{\partial p_t}&=\mathrm{S}(t)\frac{\partial}{\partial p}\mathrm{S}(t)^{-1}\ ,\quad \frac{\partial}{\partial q_t}=\mathrm{S}(t)\frac{\partial}{\partial q}\mathrm{S}(t)^{-1}\ . \end{aligned} \tag{4.16}$$

Thus, by differentiating (4.14) with respect to t, we obtain

$$\frac{dA_s(t;\,p,q)}{\partial t}=-i\mathrm{S}(t)\mathscr{L}(p,q,t)A_s(p,q)$$
$$=-i\mathrm{S}(t)\mathscr{L}(p,q,t)\mathrm{S}(t)^{-1}\mathrm{S}(t)A_s(p,q)$$
$$=-i\mathscr{L}(p_t,q_t,t)A_s(t;\,p,q)\,,$$

which proves that (4.14) is the solution of (4.12) and at the same time that it is equal to (4.8).

If the density operater represents the canonical distribution with the parameter

$$\beta=1/kT\,,$$

it satisfies the Bloch equation,

$$\frac{\partial}{\partial\beta}\rho=-\mathscr{H}\rho\,, \tag{4.17a}$$

or

$$\frac{\partial}{\partial\beta}\rho=-\rho\mathscr{H}\,, \tag{4.17b}$$

with the initial condition,

$$\rho_{\beta=0}=\mathbf{1}\,.$$

The Bloch equation, (4.17a) or (4.17b), is interpreted into the Wigner representation as

$$\frac{\partial f}{\partial\beta}=-\mathscr{H}_w f\,, \tag{4.18a}$$

or

$$\frac{\partial f}{\partial\beta}=-\bar{\mathscr{H}}_w f\,. \tag{4.18b}$$

Therefore the Wigner d. f. for the canonical distribution satisfies

$$\frac{\partial f}{\partial\beta}=-\frac{1}{2}(\mathscr{H}_w+\bar{\mathscr{H}}_w)\,,$$
$$\equiv-\frac{1}{2}\{\mathscr{H}(p_w,q_w)+\mathscr{H}(\bar{p}_w,\bar{q}_w)\}f\,. \tag{4.19}$$

Thus, it can be written as

$$f(p,q;\,\beta)=e^{-\beta\mathscr{H}_w}\cdot 1$$
$$=e^{-\beta\bar{\mathscr{H}}_w}\cdot 1$$
$$=e^{-\beta(\mathscr{H}_w+\bar{\mathscr{H}}_w)/2}\cdot 1\,. \tag{4.20}$$

Any of these expressions can be used for computation.

Part II. Electrons in a Magnetic Field

§ 5. Commutation Rules and Wigner Representation

Let us now consider an electron in a magnetic field $\vec{H}$ which is derived from a vector potential $\vec{A}(\vec{x})$. The Hamiltonian is then given by

$$\mathscr{H}=\frac{1}{2m}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2+V(\vec{x})\,, \tag{5.1}$$

where $\vec{p}$ is the canonical momentum. The physical momentum $\vec{\pi}$ may be defined by

$$\vec{\pi}\equiv m\frac{d\vec{x}}{dt}=\vec{p}-\frac{c}{c}\vec{A}\,, \tag{5.2}$$

which satisfy the commutation rules

$$[\pi_x,\pi_y]=-\frac{\hbar e}{ic}\left\{\frac{\partial A_y}{\partial x}-\frac{\partial A_x}{\partial y}\right\}=-\frac{\hbar e H_z}{ic}\,, \tag{5.3}$$

and

$$[\pi_x,x]=\frac{\hbar}{i}\,,\quad\text{etc.} \tag{5.4}$$

We shall use in the following the variables, $\vec{\pi}$ and $\vec{x}$, instead of $\vec{p}$ and $\vec{x}$. These are not canonical since they have the extra non-vanishing commutator (5.3), but they are independent of the gauge of the vector potential and have the advantage of being more physical than the canonical variables $\vec{p}$ and $\vec{x}$. In terms of these variables, the Hamiltonian (5.1) keeps the form,

$$\mathscr{H}=\frac{1}{2m}\vec{\pi}^2+V(\vec{x})\,, \tag{5.5}$$

the magnetic field entering only into the commutator (5.3).

Now, a Wigner distribution function, originally defined as a function of $\vec{p}$ and $\vec{x}$, can be regarded as a function of $\vec{\pi}$ and $\vec{x}$ simply by the change of independent variables defined by (5.2), which has the Jacobian equal to 1; i. e.

$$\frac{\partial(\pi_x,\pi_y,\pi_z,x,y,z)}{\partial(p_x,p_y,p_z,x,y,z)}=1\,.$$

Then any Wigner operator, introduced for the $p-x$ representation of Wigner distribution functions can be transformed into a differential operator operating on functions of $\vec{\pi}$ ond $\vec{x}$. By changing the independent variables in this way, we have the transformation,

$$\frac{\partial}{\partial p_x}=\frac{\partial}{\partial\pi_x}\,,\quad\text{etc.,} \tag{5.6}$$

$$\left(\frac{\partial}{\partial x}\right)_p=\left(\frac{\partial}{\partial x}\right)_\pi-\frac{e}{c}\left(\frac{\partial A_x}{\partial x}\frac{\partial}{\partial\pi_x}+\frac{\partial A_y}{\partial x}\frac{\partial}{\partial\pi_y}+\frac{\partial A_z}{\partial x}\frac{\partial}{\partial\pi_z}\right)\,,\quad\text{etc..}$$

Thus we have the following transformation of the Wigner operators:

$$x_w\equiv x-\frac{\hbar}{2i}\frac{\partial}{\partial p_x}=x-\frac{\hbar}{2i}\frac{\partial}{\partial\pi_x}\,,\quad\text{etc.} \tag{5.7}$$

$$\pi_{xw}\equiv p_x+\frac{\hbar}{2i}\frac{\partial}{\partial x}$$
$$-\frac{e}{c}A_x\left(x-\frac{\hbar}{2i}\frac{\partial}{\partial p_x},\ y-\frac{\hbar}{2i}\frac{\partial}{\partial p_y},\ z-\frac{\hbar}{2i}\frac{\partial}{\partial p_z}\right)$$
$$=\pi_x+\frac{\hbar}{2i}\frac{\partial}{\partial x}$$
$$-\frac{\hbar e}{2ic}\left(\frac{\partial A_x}{\partial x}\frac{\partial}{\partial \pi_x}+\frac{\partial A_y}{\partial x}\frac{\partial}{\partial \pi_y}+\frac{\partial A_z}{\partial x}\frac{\partial}{\partial \pi_z}\right)$$
$$+\frac{e}{c}\Big\{A_x(x, y, z)$$
$$-A_x\left(x-\frac{\hbar}{2i}\frac{\partial}{\partial \pi_y},\ y-\frac{\hbar}{2i}\frac{\partial}{\partial \pi_x},\ z-\frac{\hbar}{2i}\frac{\partial}{\partial \pi_z}\right)\Big\}, \quad \text{etc.} \tag{5.8}$$

If the magnetic field is varying in space only slowly, the last term of (5.8) can be expanded to result in

$$\pi_{xw}=\pi_x+\frac{\hbar}{2i}\frac{\partial}{\partial x}$$
$$-\frac{\hbar e}{2ic}\left(H_z\frac{\partial}{\partial \pi_y}-H_y\frac{\partial}{\partial \pi_z}\right), \text{ etc.} \tag{5.9}$$

which is exact if $\vec{H}$ is uniform or is a good approximation if

$$\hbar|\operatorname{grad} H|/H \ll |\pi| , \tag{5.10}$$

for relevant values of the momentum, i. e., if the magnetic field hardly changes in the characteristic wave length of the electron.

Thus we can define a Wigner representation for the quantum mechanics of electrons in a magnetic field, which may be called the $(\vec{\pi}, \vec{x})$ Wigner representation. Unlike the Wigner representation discussed in Part I, this is characterized by the use of noncanonical variables. It is rather important from a general methodological point of view to recognize that noncanonical variables can be introduced in the Wigner representation in such a simple manner.

Let us assume a uniform, constant magnetic field $\vec{H}$, for which (5.9) holds exactly. The equation of motion of the density matrix will be written in the $(\vec{\pi}, \vec{x})$ Wigner representation as

$$\frac{\partial}{\partial t}f(\vec{\pi}, \vec{x}, t)=i\mathscr{L}_H f(\vec{\pi}, \vec{x}, t) , \tag{5.11}$$

where

$$i\mathscr{L}_H=\frac{1}{i\hbar}\{\mathscr{H}(\vec{\pi}_w, \vec{x}_w)-\mathscr{H}(\bar{\vec{\pi}}_w, \bar{\vec{x}}_w)\}$$
$$=-\frac{1}{m}\vec{\pi}\frac{\partial}{\partial \vec{x}}$$
$$+\frac{1}{i\hbar}\left\{V\left(\vec{x}-\frac{\hbar}{2i}\frac{\partial}{\partial\vec{\pi}}\right)-V\left(\vec{x}+\frac{\hbar}{2i}\frac{\partial}{\partial\vec{\pi}}\right)\right\}$$
$$+\frac{e}{c}\vec{H}\cdot\vec{\pi}\times\frac{\partial}{\partial\vec{\pi}} . \tag{5.12}$$

The quantum mechanical Liouville operator, $i\mathscr{L}_H$, in this representation takes a particularly simple form. The first two terms of (5.12), i. e.,

$$i\mathscr{L}=-\frac{1}{m}\vec{\pi}\frac{\partial}{\partial\vec{x}}+\frac{1}{i\hbar}\{V_w-\bar{V}_w\} , \tag{5.13}$$

is exactly the same as that in the absence of a magnetic field, while the last term

$$i\mathscr{L}'=\frac{e}{mc}\vec{H}\cdot\vec{\pi}\times\frac{\partial}{\partial\vec{\pi}}=\omega_c\left(\pi_x\frac{\partial}{\partial\pi_y}-\pi_y\frac{\partial}{\partial\pi_x}\right) , \tag{5.14}$$

represents the Lorentz force. The last expression is for the case where $\vec{H}$ lies in the z-direction, ω_c being the cyclotron frequency

$$\omega_c=eH/mc . \tag{5.15}$$

Note that (5.14) is very simple because of the assumption of a constant mass m in (5.1). This is one of the advantages of using a Wigner representation in a magnetic problem.

§ 6. Landau Diamagnetism

As an illustration of the application of the Wigner representation in magnetic problems let us here consider the diamagnetism of electrons. For simplicity, we ignore the electron interactions so that the problem is essentially a one-particle problem. First we treat non-degenerate electrons obeying the Boltzmann statistics. Degenerate cases can easily be obtained from the results of a non-degenerate case.

Therefore, we now calculate the density matrix

$$\rho=e^{-\beta\mathscr{H}} , \tag{6.1}$$

in the $(\vec{\pi}, \vec{x})$ Wigner representation. The Wigner d. f. is then given by

$$f(\vec{\pi}, \vec{x})=e^{-\beta\mathscr{H}_w}\cdot 1 , \tag{6.2}$$

where the Wigner operator H_w is given by

$$\mathscr{H}_w=\frac{1}{2m}\vec{\pi}_w{}^2+V_w=\mathscr{H}_w{}^0+\mathscr{H}_w{}'+\mathscr{H}_w{}''$$
$$\mathscr{H}_w{}^0=\frac{1}{2m}\left\{\left(\pi_x+\frac{\hbar}{2i}\frac{\partial}{\partial x}\right)^2+\left(\pi_y+\frac{\hbar}{2i}\frac{\partial}{\partial y}\right)^2\right.$$
$$\left.+\left(\pi_z+\frac{\hbar}{2i}\frac{\partial}{\partial z}\right)^2\right\}$$

$$+V\left(x-\frac{\hbar}{2i}\frac{\partial}{\partial\pi_x},\quad y-\frac{\hbar}{2i}\frac{\partial}{\partial\pi_y},\quad z-\frac{\hbar}{2i}\frac{\partial}{\partial\pi_z}\right),\tag{6.3}$$

$$\mathscr{H}_w'=-\frac{\hbar'}{2mi}\left\{\left(\pi_x+\frac{\hbar}{2i}\frac{\partial}{\partial x}\right)\frac{\partial}{\partial\pi_y}-\left(\pi_y+\frac{\hbar}{2i}\frac{\partial}{\partial\pi_x}\right)\frac{\partial}{\partial y_x}\right\}$$

$$\mathscr{H}_w''=-\frac{\hbar'^2}{8m}\left(\frac{\partial^2}{\partial\pi_x{}^2}+\frac{\partial^2}{\partial\pi_y{}^2}\right).\tag{6.4}$$

The magnetic field H is assumed to be in the z-direction and $\hbar'$ is defined by

$$\hbar'=eH\hbar/c\,.\tag{6.5}$$

In order to calculate f to the first order of H, $\mathscr{H}_w''$ in (6.3) may be omitted, and (6.2) can be expanded in $\mathscr{H}_w'$ as

$$f(\vec\pi,\vec x)=f^0(\vec\pi,\vec x)+f'(\vec\pi,\vec x)+\cdots$$
$$=\left\{e^{-\beta\mathscr{H}^0{}_w}-\int_0^\beta d\lambda e^{-(\beta-\lambda)\mathscr{H}_w{}^0}\mathscr{H}_w'e^{-\lambda\mathscr{H}_w{}^0}\cdots\right\}1\tag{6.6}$$

As is well known, in the limit of $\hbar\to0$, the classical electrons will not give any magnetic effect. If the spins of electrons are disregarded the lowest order quantum effect starts from the order $\hbar^2$, which is the Landau diamagnetism. This is obtained from (6.6) by a very simple calculation in the following way.

Note first that

$$e^{-\lambda\mathscr{H}^0{}_w}\cdot1=e^{-\lambda\mathscr{H}_0}+O(\hbar^2),\tag{6.7}$$

where

$$\mathscr{H}_0=\frac{1}{2m}\vec\pi^2+V(\vec x)\,.$$

The fact that a Wigner d. f. contains $\hbar$ only in even powers is immediately seen from (4.19). Since $\mathscr{H}_w'$ is already $O(\hbar)$, the same classical limit can be used in exp $\{-(\beta-\lambda)\mathscr{H}_w{}^0\}$ in (6.6). Thus we easily obtain

$$f'(\vec\pi,\vec x)=\frac{\hbar'}{2mi}\int_0^\beta dx\,e^{-(\beta-\lambda)\mathscr{H}_0}$$
$$\times\left\{\left(\pi_x+\frac{\hbar}{2i}\frac{\partial}{\partial x}\right)\frac{\partial}{\partial\pi_y}-\left(\pi_y+\frac{\hbar}{2i}\frac{\partial}{\partial y}\right)\frac{\partial}{\partial\pi_x}\right\}e^{-\lambda\mathscr{H}_0}$$
$$=-\frac{\hbar\hbar'}{4m}\int_0^\beta d\lambda\cdot\lambda^2\left(\frac{\pi_y}{m}\frac{\partial V}{\partial x}-\frac{\pi_x}{m}\frac{\partial V}{\partial y}\right)e^{-\beta\mathscr{H}_0}$$
$$=-\frac{\hbar\hbar'}{12m^2}\beta^3\left(\pi_y\frac{\partial V}{\partial x}-\pi_x\frac{\partial V}{\partial y}\right)e^{-\beta\mathscr{H}_0}\,.\tag{6.8}$$

This is a good approximation for a slowly changing potential V, because the expansion of a Wigner d. f. in $\hbar$ as (6.7) is essentially an expansion in terms of the ratio of the relevant electron wave length and a length characterizing the spacial variation of V.

The current distribution is obtained by

$$j_x=-\frac{e}{m}\int\pi_xf'(\vec\pi,\vec x)d\vec\pi\Big/\int f(\vec\pi,\vec x)d\vec\pi\,.\tag{6.9}$$

By using (6.8) and (6.7) we obtain the current density distribution in $O(\hbar^{-2})$ as

$$\vec j(\vec x)=-\frac{N\hbar^2e^2\beta^2}{12m^2c}(\vec H\times\mathrm{grad}\,V)e^{-\beta V}\Big/\int e^{-\beta V}d\vec x\tag{6.10}$$

or

$$\vec j(\vec x)=c\frac{\beta}{3}\mu_B{}^2\vec H\times\mathrm{grad}\,n(\vec x)\,,\tag{6.11}$$

where N is the total number of electrons, $n(\vec x)$ their density at $\vec x$ and μ_β is the Bohr magneton. The magnetic moment density $\vec m(\vec x)$ is then given by

$$\vec m(\vec x)=-\frac{\beta}{3}\mu_B{}^2n(\vec x)\cdot\vec H\,,\tag{6.12}$$

and the total magnetic moment $\vec\mu$ by

$$\vec\mu=-\frac{N}{3}\beta\mu_B{}^2\vec H\equiv-\frac{N\mu_B{}^2}{3kT}\vec H\,,\tag{6.13}$$

which is the Landau diamagnetism for obtained by nondegenerate electrons. This may also be calculating the moment of current distribution from (6.11), using the virial theorem,

$$\left\langle x\frac{\partial V}{\partial x}\right\rangle=\left\langle y\frac{\partial V}{\partial y}\right\rangle=kT\,,\tag{6.14}$$

which holds in the Boltzmann statistics irrespective of the potential.

The above results can be easily translated into degenerate Fermi statistics with the aid of the operator equation,

$$g(\mathscr{H})=\int g(E)dE\delta(E-\mathscr{H})$$
$$=\int g(E)dE\frac{1}{2\pi i}\int e^{\beta E-\beta\mathscr{H}}d\beta\,.\tag{6.15}$$

Thus, for example

$$f_F(\vec\pi,\vec x;\beta)=\int\frac{dE}{e^{\beta(E-\zeta)}+1}\frac{1}{2\pi i}\int f_B(\vec\pi,\vec x;\beta)e^{\beta E}d\beta',\tag{6.16}$$

gives the Wigner d. f. for electrons obeying the Fermi statistics if the unnormalized Boltzmann-Wigner d. f. $f(\vec\pi,\vec x)$, Eq. (6.6), is inserted into f_B in the integrand. Similarly, expectations of physical quantities can be obtained from the results for the Boltzmann statistics. For instance, the current density (6.11) can be translated into that for the Fermi-distribution as

$$\vec{j}_F(\vec{x})=\frac{1}{3}c\mu_B{}^2\vec{H}\times\text{grad}\, n_F(\vec{x})\ , \tag{6.17}$$

where

$$n_F(\vec{x})=\frac{1}{h^3}\iint\delta'\left(E-\frac{\vec{\pi}^2}{2m}-V(\vec{x})\right)d\vec{\pi}dEg(E)\ , \tag{6.18}$$

$g(E)$ being the Fermi distribution function. For strongly degenerate electrons, this becomes

$$n_F(\vec{x})=\frac{1}{h^3}\int\delta\left(\zeta-\frac{\vec{\pi}^2}{2m}-V(\vec{x})\right)d\vec{\pi}\ , \tag{6.19}$$

which is an approximation for a slowly varying potential as is obtained by a WKB approximation. The integrated magnetic moment is then given by

$$\vec{\mu}=-\frac{1}{3}\mu_B{}^2\,\Omega(\zeta)\vec{H}\ , \tag{6.20}$$

for degenerate electrons, $\Omega(\zeta)$ being the state density at the Fermi level ζ. Equation (6.20) is the well known result of Landau diamagnetism.

A few points may be remarked here. The expressions (6.13) or (6.20) for the Landau diamagnetism of non-interacting electrons can be derived in different ways. First, one may calculate the free energy of electrons in a free space ($V=0$) by considering the quantized Landau levels[5]. The free energy increases in H^2 corresponding to the diamagnetism. Also, one can obtain the same result for completely free electrons in a non-uniform magnetic field, by taking a limit of susceptibility as the wave-length of the imposed field grows to infinity. These derivations seem to indicate that the Landau diamagnetism is a bulk property and exists even for free electrons. On the other hand, Eqs. (6.10) and (6.17) show that the diamagnetic current exists only when the potential is varying in space.

The current flows in perpendicular to the potential gradient or along the equipotential lines. Although these formulae apply only for a slowly varying potential, not for an abruptly changing potential, this feature of the diamagnetic current is generally true. Landau[6] showed this by calculating the current along the circumference of the domain confining free electrons. This gives an interpretation of the Landau diamagnetism as a surface effect.

These two interpretations of the Landau diamagnetism are not contradictory, because a surface integral may be transformed into a volume integral. However, it seems important to realize that the Landau diamagnetism is associated with a current which arises from a sort of quantum fluctuation directed by the potential gradient and the applied magnetic field. This a physical interpretation of Eq. (6.10).

The present treatment can be extended to include the electron spins and the spin-orbit coupling effect. For that purpose the Wigner d. f., (6.2), is regarded as a two-component vector and the Wigner operators are regarded as two-by-two matrices corresponding to the spin operators. It is easy to see, then, that to $0(\hbar^2)$ the orbital part and the spin part are simply additive in the magnetic susceptibility. The contribution of orbital paramagnetism also enters only from $0(\hbar^4)$. It seems to be very interesting to apply this method to the study of orbital and spin magnetism of impurity states in metals. Details of such an application will be reported later.

When the potential V is rapidly changing in space, the wave nature of electron motion will predominate so that an expansion of $f(\vec{\pi},\vec{x})$, (6.2), in $\hbar$, is not convenient. The use of the Wigner representation in the form as described in §5 is not, however, intended to be necessarily bound to such an expansion. It is rather meant to be used for an expansion in $\hbar'$, (6.5), or in the magnetic field. Thus, it is sometimes advisable to use this representation only for such a purpose and to switch back to ordinary quantum mechanical representation.

For instance, Eq. (6.6) gives

$$f'(\vec{\pi},\vec{x})=\frac{\hbar'}{2mi}\int_0^\beta e^{-(\beta-\lambda)\mathscr{H}_0}\times\left\{\left(\pi_x+\frac{\hbar}{2i}\frac{\partial}{\partial x}\right)\frac{\partial}{\partial\pi_y}-\left(\pi_y+\frac{\hbar}{2i}\frac{\partial}{\partial y}\right)\frac{\partial}{\partial\pi_x}\right\}\times e^{-\lambda\mathscr{H}_w{}^0}\cdot|\ , \tag{6.21}$$

for the first order (in H) deviation of the Wigner d. f. The corresponding quantum operator can be easily found by using the rule stated by the theorem 4 in §3. This is given by*

$$\rho'=-\frac{\omega_c}{2}\int_0^\beta d\lambda e^{-(\beta-\lambda)\mathscr{H}_0}$$
$$\times\{p_x[y, e^{-\lambda\mathscr{H}_0}]-p_y[x, e^{-\lambda\mathscr{H}_0}]\}, \quad (6.22)$$

where the momentum is now written as $\vec{p}$ because the Hamiltonian $\mathscr{H}_0$ does not involve the magnetic field and so there is no distinction between $\vec{p}$ and $\vec{\pi}$. In (6.22), the position variables x and y appear in commutators with a density operator, because they correspond to the differential operator

$$-\frac{\hbar}{i}\frac{\partial}{\partial\pi_x}=x_w-\bar{x}_w, \quad -\frac{\hbar}{i}\frac{\partial}{\partial\pi_y}=y_w-\bar{y}_w,$$

which appear in (6.21).

The average orbital magnetic moment is obtained from ρ'; i. e.

$$\bar{\mu}=-\frac{e\omega^p}{4mcZ_0}\operatorname{Tr} L_z\int_0^\beta d\lambda e^{-(\beta-\lambda)\mathscr{H}_0}$$
$$\times\{p_x[ye^{-\lambda\mathscr{H}_0}]-p_y[xe^{-\lambda\mathscr{H}_0}]\}, \quad (6.23)$$

where Z_0 is the partition

$$Z_0=\operatorname{Tr} e^{-\beta\mathscr{H}_0},$$

and L_z is the angular momentum in z-direction. Eq. (6.23) can be transformed into

$$\bar{\mu}=\frac{e^2H}{4m^2c^2Z_0}$$
$$\times\operatorname{Tr}\left\{\int_0^\beta d\lambda e^{-(\beta-\lambda)\mathscr{H}_0}L_z e^{-\lambda\mathscr{H}_0}L_z\right.$$
$$\left.-e^{-\beta\mathscr{H}_0}m(x^2+y^2)\right\}, \quad (6.24)$$

which is a familiar expression of the orbital magnetic moment. For this transformation we use the relation

$$\operatorname{Tr}\int_0^\beta d\lambda e^{-(\beta-\lambda)\mathscr{H}_0}p_x e^{-\lambda\mathscr{H}_0}yL_z$$
$$=\operatorname{Tr}\frac{m}{i\hbar}[e^{-\beta\mathscr{H}_0}, x]yL_z$$
$$=\frac{m}{i\hbar}\operatorname{Tr} e^{-\beta\mathscr{H}_0}[x, yL_z]=m\operatorname{Tr} e^{-\beta\mathscr{H}_0}y^2,$$

and a similar equation

$$\operatorname{Tr}\int_0^\beta d\lambda e^{-(\beta-\lambda)\mathscr{H}_0}p_y e^{-\lambda\mathscr{H}_0}xL_z$$
$$=m\operatorname{Tr} e^{-\beta\mathscr{H}_0}x^2,$$

which are obtained by the identity[6)]

$$\int_0^\beta d\lambda e^{-(\beta-\lambda)\mathscr{H}_0}\dot{A}e^{-\lambda\mathscr{H}}=[e^{-\beta\mathscr{H}}, A].$$

The expression of ρ', (6.22), may also be written as

$$\rho'=-\frac{\omega_c}{2}\int_0^\beta dx\{[e^{-(\beta-\lambda)\mathscr{H}_0}, y]p_x$$
$$-[e^{-(\beta-\lambda)\mathscr{H}_0}, x]p_y\}e^{-\lambda\mathscr{H}_0}$$
$$=-\frac{\omega_c}{2}\int_0^\beta d\lambda\{[e^{-\lambda\mathscr{H}_0}, y]p_x$$
$$-[e^{-\lambda\mathscr{H}_0}, x]p_y\}e^{-(\beta-\lambda)\mathscr{H}_0}. \quad (6.25)$$

The difference of this and (6.22) is

$$\frac{\omega_c}{2}\int_0^\beta d\lambda\{[e^{-(\beta-\lambda)\mathscr{H}_0}p_x e^{-\lambda\mathscr{H}_0}, y]$$
$$-[e^{-(\beta-\lambda)\mathscr{H}_0}p_z e^{-\lambda\mathscr{H}_0}, x]\}$$
$$=\frac{m\omega_c}{2i\hbar}\{[[e^{-\beta\mathscr{H}_0}, x]y]-[[e^{-\beta\mathscr{H}_0}y]x]\}$$
$$=\frac{m\omega_c}{2i\hbar}[e^{-\beta\mathscr{H}_0}[x, y]]=0.$$

Thus ρ' can be written as

$$\rho'=-\frac{\omega_c}{4}\int_0^\beta d\lambda\{[e^{-(\beta-\lambda)\mathscr{H}_0}, y]p_x e^{-\lambda\mathscr{H}_0}$$
$$+e^{-\lambda\mathscr{H}_0}p_x[y, e^{-(\beta-\lambda)\mathscr{H}_0}]$$
$$-[e^{-(\beta-\lambda)\mathscr{H}_0}, x]p_y e^{-\lambda\mathscr{H}_0}$$
$$-e^{-\lambda\mathscr{H}_0}p_y[x, e^{-(\beta-\lambda)\mathscr{H}_0}]\}, \quad (6.26)$$

which exhibits clearly the hermitian property of ρ'.

Generally, the two terms in (6.24) have a big cancellation which, of course, must arise because the second term becomes large if the electron distribution extends in space. The expression of ρ' in (6.22) or (6.26) makes this cancellation appear in a more natural way. Therefore, these equations and (6.23) will be useful for calculation of the orbital magnetism.

§ 7. Application to Electronic Conduction

Eq. (5.11) can be conveniently applied to the problem of electronic conduction. When an external electric field $\vec{E}$ is applied, Eq. (5.11) takes the form

$$\frac{\partial f}{\partial t}=i(\mathscr{L}_0+\mathscr{L}'+\mathscr{L}_{\text{ext}})f\equiv i(\mathscr{L}+\mathscr{L}_{\text{ext}})f, \quad (7.1)$$

where

$$i\mathscr{L}_0=-\Sigma\frac{\pi}{m}\frac{\partial}{\partial x}+\frac{1}{i\hbar}(V_w-\bar{V}_w), \quad (7.2)$$

V being the internal potential

* In this and following sections quantum operators are denoted simply by italic letters in stead of gothic letters when they are written in more or less familiar quantum-mechanical expressions.

$$i\mathscr{L}'=\omega_c\sum\left(\pi_x\frac{\partial}{\partial\pi_y}-\pi_y\frac{\partial}{\partial\pi_x}\right), \qquad (7.3)$$

and

$$i\mathscr{L}_{\text{ext}}=e\vec{E}\sum\frac{\partial}{\partial\vec{\pi}}. \qquad (7.4)$$

The summation is carried over electrons. Following the general method as given by the author[7], Eq. (7.1) can be solved to the first order of the external field, which is assumed to be weak, starting from the condition,

$$\vec{E}(t)\to 0 \quad \text{as } t\to-\infty,$$
$$f\to f_e \quad \text{(equilibrium)}.$$

Then we have

$$f-f_e\equiv\Delta f$$
$$=\int_{-\infty}^{t}dt' e^{i\mathscr{L}(t-t')}i\mathscr{L}_{\text{ext}}(t')f_e, \qquad (7.5)$$

from which the electric current is calculated by

$$j_\mu(t)=-\int d\Gamma\sum\frac{e\pi_\mu}{m}$$
$$\times\int_{-\infty}^{t}dt' e^{i\mathscr{L}(t-t')}i\mathscr{L}_{\text{ext}}(t')f_e, \qquad (7.6)$$

where $\int d\Gamma$ is the phase space integration. Inserting (7.4) in (7.6) we obtain the conductivity in the form

$$\sigma_{\mu\nu}(\omega)=\int_0^\infty e^{-i\omega t}dt\phi_{\mu\nu}(t), \qquad (7.6)$$

$$\phi_{\mu\nu}(t)=-\frac{e^2}{m}\int d\Gamma\sum\pi_\mu e^{i\mathscr{L}t}\sum\frac{\partial}{\partial\pi_\nu}f_e. \qquad (7.7)$$

This may be transformed into

$$\phi_{\mu\nu}(t)=\frac{e^2}{m}\int d\Gamma f_e\sum\frac{\partial}{\partial\pi_\nu}e^{-\mathscr{L}t}\sum\pi_\mu, \qquad (7.8)$$

by partial integration. Eq. (7.7) or (7.8) is equivalent to

$$\phi_{\mu\nu}(t)=\frac{e^2}{mi\hbar}\operatorname{Tr}\rho_e[\sum x_\nu, \sum\pi_\mu(t)]$$
$$=\frac{e^2}{m^2}\int_0^\beta d\lambda\operatorname{Tr}\rho_e e^{\lambda\mathscr{H}}\sum\pi_\nu e^{-\lambda\mathscr{H}}\sum\pi_\mu(t). \qquad (7.9)$$

Let us now use (7.7) to obtain an expansion in the magnetic field. This can be done by using (7.9), but Eq. (7.7) is more convenient for this purpose. Since the magnetic field appears in $\mathscr{L}$ as $\mathscr{L}'$, we easily make the expansion,

$$\phi_{\mu\nu}(t)=-\frac{e^2}{m}\int d\Gamma\sum\pi_\mu e^{i\mathscr{L}_0t}$$
$$\times\left\{1+\int_0^t dt' e^{-\mathscr{L}_0t'}i\mathscr{L}'e^{i\mathscr{L}_0t'}+\cdots\right\}$$
$$\times\sum\frac{\partial}{\partial\pi_\nu}(f^0+f'+\cdots). \qquad (7.10)$$

For simplicity we consider here only the first order term in H, which consists of two terms:

$$\phi'_{\mu\nu}(t)=\phi'_{\mu\nu,1}(t)+\phi'_{\mu\nu,2}(t), \qquad (7.11)$$

where

$$\phi'_{\mu\nu,1}(t)=-\frac{e^2}{m}\int d\Gamma\sum\pi_\mu$$
$$\times\int_0^t dt' e^{i\mathscr{L}_0(t-t')}i\mathscr{L}'e^{i\mathscr{L}_0t'}\sum\frac{\partial}{\partial\pi_\nu}f^0, \qquad (7.12)$$

$$\phi'_{\mu\nu,2}(t)=-\frac{e^2}{m}\int d\Gamma\sum\pi_\mu e^{i\mathscr{L}_0t}\sum\frac{\partial}{\partial\pi_\nu}f'. \qquad (7.13)$$

The first term (7.12) is the effect of magnetic field on the electron motion in the conduction process, while the second term (7.13) originates from the change of equilibrium electron distribution in the magnetic field. As was discussed in the previous section, the latter is purely a quantum-mechanical effect whereas the former is present even in the classical limit. This difference seems an important point.

More explicitly, (7.12) is written as

$$\phi'_{xy,1}=-\frac{e^2\omega_c}{m}\int_0^t d\Gamma\sum\pi_x\int_0^t dt' e^{i\mathscr{L}_0(t-t)'}$$
$$\times\sum\left(\pi_x\frac{\partial}{\partial\pi_y}-\pi_y\frac{\partial}{\partial\pi_x}\right)e^{i\mathscr{L}_0t'}\sum\frac{\partial}{\partial\pi_y}f^0, \qquad (7.14)$$

or in ordinary quantum operators

$$\phi'_{xy,1}=-\frac{e^2\omega_c}{i\hbar m}\int_0^t dt'\operatorname{Tr}\rho_0$$
$$\times\left[\sum y, \sum\left\{\pi_x(t'), \frac{1}{i\hbar}[y(t'), \sum\pi_x(t)]\right\}\right.$$
$$\left.-\sum\left\{\pi_y(t'), \frac{1}{i\hbar}[x(t'), \sum\pi_x(t)]\right\}\right]$$
$$=\frac{e^2\omega_c}{m^2}\int_0^t dt'\operatorname{Tr}\rho_0\int_0^\beta d\lambda e^{\lambda\mathscr{H}_0}\sum\pi_y e^{-\lambda\mathscr{H}_0}$$
$$\times\left(\sum\left\{\pi_x(t')\left[\frac{1}{i\hbar}y(t'), \pi_x(t)\right]\right\}\right.$$
$$\left.-\sum\left\{\pi_y(t')\left[\frac{1}{i\hbar}x(t'), \pi_x(t)\right]\right\}\right), \qquad (7.15)$$

where $\{A, B\}$ means a symmetrixed product of A and B. Similarly, (7.13) is written as

$$\phi'_{xy,2}(t)=\frac{\hbar e^2\omega_c}{2mi}\int d\Gamma\sum\pi_x e^{i\mathscr{L}_0t}\sum\frac{\partial}{\partial\pi_y}f', \qquad (7.16)$$

$$=\frac{e^2\omega_c}{Z_0 2mi\hbar}\mathrm{Tr}\Big[\sum y,\ \int_0^\beta d\lambda e^{-(\beta-\lambda)\mathscr{H}_0}$$

$$(\sum p_x[y,\ e^{-\lambda\mathscr{H}_0}]-\sum p_y[x,\ e^{-\lambda\mathscr{H}_0}])\Big]\sum\pi_x(t)$$

$$=\frac{e^2\omega_c}{2mZ_0}\int_0^\beta d\lambda\ \mathrm{Tr}\, e^{-(\beta-\lambda)\mathscr{H}_0}\sum(p_x[y,\ e^{-\lambda\mathscr{H}_0}]$$

$$-p_y[x,\ e^{-\lambda\mathscr{H}_0}]\frac{1}{i\hbar}[\sum y,\ \sum\pi_x(t)]\Big]. \qquad (7.17)$$

These expressions may be used for a systematic study of the Hall constant, which is now under way and will be reported elsewhere.

Here we make only a brief remark on the magnetic field effect on the conductivity. If the equilibrium distribution f^0 in (7.14) is symmetric in π_x and π_y, then we expect that

$$\sum\frac{\partial}{\partial\pi_y}f^0\propto\sum\pi_y f^0 .$$

This means that, by an electric field pulse applied in the y-direction, the distribution of electrons is shifted in the momentum space giving rise to a deviation characterized by a Y_1–spherical harmonics. The expression (7.14) is then interpreted in the following way: This deviation propagates in time from $t=0$ to t', and then it feels the Lorentz force from the magnetic field. If the deviation still keeps its Y_1–character, the direction of Y_1–harmonics is then turned by 90°. From t' to t, the distribution function changes without the effect of magnetic field. At the time t, the current is measured in the x-direction. The intermediate time t' is chosen between 0 and t and the integrated result of the abovementioned process is the first order effect in the response function. From this interpretation, it is clear that we would have

$$\phi'_{xy,1}(t)=-\omega_c t\phi_{yy}(t) . \qquad (7.18)$$

This is true, however, only if the propagation in $(0,\ t')$ and that in $(t',\ t)$ are totally uncorrelated. Such an assumption may be allowed either if the electrons are scattered by very local scatterers or if the scattering potential is so weak that any higher order correlation may be neglected. Equation (7.18) yields, in the ideal case of

$$\phi_{xx}(t)=\phi_{yy}(t)=\frac{e^2n}{m}e^{-t/\tau} ,$$

$$\sigma_{xy}=-\frac{e^2n}{m}\omega_c\tau^2=-\sigma_{xx}\omega_c\tau . \qquad (7.19)$$

Thus, the ideal form of σ_{xy}, (7.19), holds only in such ideal limits. If the force range of scattering potential becoms larger, so that the ratio

T_d/T_f=duration of collision/mean free time becomes larger, deviations from (7.19) are generally to be expected.

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